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X-RAY ABSORPTION ANALYSIS OF STRUCTURAL DISORDER IN AMORPHOUS SILICON

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Abstract. *Different levels of order of amorphous silicon (a-Si) samples have been measured by XANES (X-ray Absorption Near Edge Structure) and EXAFS (Extended X-ray Absorption Fine structure) analysis. The EXAFS analysis has been carried out by using a first-shell fitting procedure while in the XANES part we have extracted the high-frequency residuals which change with the level of order. From this analysis a continuous increase of local ordering has been found as a function of the substrate deposition temperature of the a-Si films.*

In this contribution we want to present a XAS (X-ray Absorption Spectroscopy) investigation on several amorphous silicon (a-Si) films prepared by using the ion beam sputtering technique. The aim of this analysis is to investigate changes in the x-ray absorption experimental spectra through a comparison with the model compound (crystalline silicon) and calculated single and multiple scattering contributions [1-3]. This analysis allows understanding of some of the characteristics of local ordering obtained increasing the substrate deposition temperature (SDT) during the growth. It is important to remark that other techniques, such as x-ray or neutron diffraction, are not able to detect differences in the local structure between a-Si samples prepared in different conditions.

Thin a-Si films (~ 1 μm) have been prepared by ion-beam sputtering for three different SDT: room temperature (RT), 200°C and 400°C. Another film was bombarded during the growth by an argon gun (Ar-B). Si K-edge EXAFS spectra with very good signal to noise ratio were recorded in transmission mode at the synchrotron radiation dedicated storage ring ACO (Orsay) by using a double InSb(111) crystal monochromator and one ionization chamber as photon detector.

The normalized modulating parts $\chi_{exp}(k)=[\alpha_{exp}(k)-\alpha_o(k)]/\alpha_o(k)$ of the absorption coefficients α_{exp} were extracted following standard procedures. Care was taken for the choice of the absorption jump and of the energy threshold E_o in order to reduce amplitude and phase errors in the fitting procedures.

The EXAFS spectra are dominated by the first-shell low-frequency contribution while a low but detectable high-frequency signal represents the contribution, mainly in the XANES part, of longer scattering paths [1,4,5,6]. In fig.1 the $\chi_{exp}(k)$ spectra of three films are shown. Apart from the main first-shell signal there are some differences in the XANES region which are shown in the panel inside the figure. The first-shell analysis was carried out by using fitting procedures in two different ways: by comparison with the crystal silicon reference signal and taking into account the calculated first-shell spectrum in the spherical wave approximation. The results are indicated in tab.1 and are consistent for both procedures. Increasing the SDT we find decreased values for the mean square relative displacements (MSRD) of the first-neighbour distances and a convergence of the mean first-shell distance to the crystalline case. There is a continuous ordering process of the first-shell local structure obtained increasing the SDT. What about the second shell?

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Sample	R(Å)	$\Delta\sigma^2$	N
RT	2.366 (6)	3.4 (6)	3.7 (2)
200	2.361 (6)	2.6 (6)	3.7 (1)
400	2.360 (6)	2.7 (7)	3.6 (2)
B-Ar	2.359 (4)	2.7 (6)	3.6 (1)

Tab.1 *Structural parameters obtained by best-fitting procedures. Here R and N are the mean first-neighbors distances and coordination numbers. $\Delta\sigma^2$ is the variation of the first-shell MSRD relative to the crystal silicon case.*

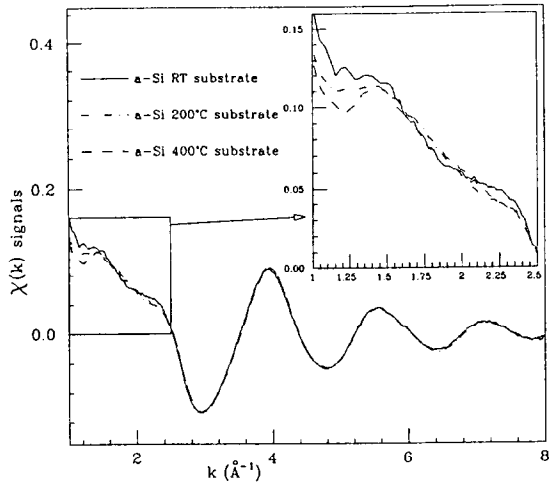

Fig.1:
$\chi_{exp}(k)$ signals of a-Si samples grown at different SDTs. The low-energy part of the spectra has been enlarged in the panel inside the figure in order to show the different behaviour of the XANES spectra, which depend on the preparation procedures.

In fig.1 differences in the x-ray absorption coefficients of the three a-Si films are shown to be detectable in a restricted region of wave vector values. In the case of the sample prepared at 400°C of SDT it is possible to detect variations up to about 4 $Å^{-1}$. These variations are mainly due to the high-frequency components of the absorption signal. Residual high-frequency signals can be easily extracted from these spectra but are difficult to analyze quantitatively. In fact, besides a damped second-shell single scattering signal, they contain also multiple (mainly double) scattering contributions. Thus the information on bond-angle disorder is shared between signals of similar amplitude but out of phase[1]. In any case the residual high-frequency signals show slight differences from one sample to another and this demonstrates that these samples have different properties of local order [7]. In particular, by fitting the difference spectra between the samples we have found that the distribution of the second-shell atoms changes going from the sample prepared at 200°C of SDT to the 400°C one. This result has been obtained by considering three calculated high-frequency signals: the second-shell single scattering signal, the two shortest double scattering group of paths which can be found inside a two-shell cluster. Therefore multiple scattering effects are shown to be essential for the interpretation of the residual high-frequency spectrum and can be used to understand the local structural properties of a-Si.

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